

Ethyl hexanoate
123-66-0 | DTXSID3021980

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 2.78 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.20e-01

Confidence level: 7.80e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Chloropyridine</div> <div>Measured: 1.81</div> <div>Predicted: 1.34</div>	<div>Image not found</div> <div>Octadecamethylcyclononasiloxane</div> <div>Measured: 2.59</div> <div>Predicted: 3.17e-05</div>	<div>Image not found</div> <div>Methyl valerate</div> <div>Measured: 3.60</div> <div>Predicted: 15.6</div>
<div>Image not found</div> <div>N-Methyldiethanolamine</div> <div>Measured: 5.96</div> <div>Predicted: 5.88e-04</div>	<div>Image not found</div> <div>Benzyl methyl ether</div> <div>Measured: 4.80</div> <div>Predicted: 1.25</div>	